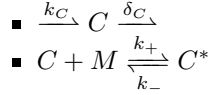


## MODEL OF BIOACCUMULATOR

### 1. MODELLING

As the Phitoquelatin is expressed linked with Omp-A we can treat it like a single complex  $C$ . So we have the reaction scheme



Where  $M$  is the free mercury and  $C^*$  is the mercury linked with the complex  $C$ ,  $k_C$  is the rate of production of the complex and  $\delta_C$  is the rate of degradation of the complex.

I will note  $[C]$  as the amount of the complex per cell,  $[C^*]$  as the amount of the complex linked with mercury per cell and  $[M]$  to the concentration of mercury, pay attention to the units.

The equation for the reactions are

$$(1) \quad \frac{d[C]}{dt} = k_C - \delta_C[C] - [C][M]k_+ + k_-[C^*]$$

$$(2) \quad \frac{d[C^*]}{dt} = [C][M]k_+ - [C^*]k_-$$

Also as the total concentration of mercury does not change we have that  $M_0 = [M] + \frac{n}{N_{Av}}[C^*]$  where  $[M]$  is the concentration of free mercury,  $n$  is the amount of cells and  $N_{Av}$  is the Avogadro's number to convert units, this last thing is for the units conversion.

$$(3) \quad \frac{d[C]}{dt} = k_C - \delta_C[C] - [C](M_0 - \frac{n}{N_{Av}}[C^*])k_+ + [C]k_-$$

$$(4) \quad \frac{d[C^*]}{dt} = [C](M_0 - \frac{n}{N_{Av}}[C^*])k_+ - [C^*]k_-$$

We can assume that the rate of splitting of the complex  $C^*$  is 0, because Mercury and Phitoquelatin have very high affinity and the degradation of the complex is very slow then  $\delta_C = 0$

$$(5) \quad \frac{d[C]}{dt} = k_C - [C](M_0 - \frac{n}{N_{Av}}[C^*])k_+$$

the interpretation of the variation of  $C$  is simple,  $k_C$  is the production term and the other thing is the consumption due to mercury binding.

$$(6) \quad \frac{d[C^*]}{dt} = [C](M_0 - \frac{n}{N_{Av}}[C^*])k_+$$

If we are at estacionaria time phase we have that the amount of cells is  $n$ , is constant, then we can say that the amount of free mercury will change as

$$(7) \quad M(t) = M_0 - \frac{n}{N_{Av}}[C^*]$$

If we are considering the exponential phase then, since bacteria grow exponentially, it is often useful to plot the logarithm of the relative population size  $[Y = \ln(N/N_0)]$  against time. So lets use the Gompertz equation to model this.

The three phases of the growth curve can be described by three parameters: the maximum specific growth rate,  $\mu_m$  is defined as the tangent in the inflection point; the lag time,  $\lambda$ , is defined as the x-axis intercept of this tangent; and the asymptote  $[A = \ln(N/N_0)]$  is the maximal value reached. Here we are not considering the death rate. [? ]

$$(8) \quad Y(t) = Ae^{-e^{\frac{\mu_m e}{A}(\lambda - t) + 1}}$$

then the equations will look like

$$(9) \quad \frac{d[C]}{dt} = k_C - [C](M_0 - \frac{e^{Y(t)}N_0}{N_{Av}}[C^*])k_+$$

$$(10) \quad \frac{d[C^*]}{dt} = [C](M_0 - \frac{e^{Y(t)}N_0}{N_{Av}}[C^*])k_+$$

where  $N_0$  is the inial cell amount, then the amount of mercury in function of time is

$$(11) \quad M(t) = M_0 - \frac{e^{Y(t)}N_0}{N_{Av}}[C^*]$$

